



## Sigma master tape, a multi-group cross section library

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Danish Atomic Energy Commission  
Research Establishment Risø

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# Sigma Master Tape, a Multi-Group Cross Section Library

by A. M. Hvidtfeldt Larsen

April 1972

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**SIGMA MASTER TAPE, a Multi-Group Cross Section Library**

by

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**Abstract**

The SIGMA MASTER TAPE is a cross section library for use in reactor physics calculations. It is generated from the UK Nuclear Data Library by the program SIGMA and contains the materials available in the UK Library, version 1968. The cross sections are given in a 78-group structure. The method of calculation and the contents of the tape are described together with the format and the use on the Borroughs B6700 computer.

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## 1. INTRODUCTION

Detailed nuclear data for reactor physics calculations are available in the form of evaluated libraries which are updated at intervals. The three main libraries, all of which are stored on magnetic tape in a form suitable for computer processing, are the ENDF/B<sup>1)</sup>, the KEDAK<sup>2)</sup> and the UKNDL<sup>3 and 4)</sup>. The present work is based on the UKNDL. By means of the processing program SIGMA the detailed data from the library are transformed into group cross sections. This, however, is a time-consuming calculation, and it was therefore decided to produce the group cross sections for relevant materials in a proper group structure once and store them on a magnetic tape which would then be the normal starting point for neutronics calculations. The SIGMA MASTER TAPE is the outcome of this procedure.

## 2. THE UKAEA NUCLEAR DATA LIBRARY

To produce the SIGMA MASTER TAPE the UKAEA Nuclear Data Library, version 1968, was used. The materials available in this version are listed in ref. 3. An updated library has been released in 1970, but as most of the modifications and additions are of minor importance for our use, it was not considered worthwhile to change to the new version. The contents of the 1970 version are listed in ref. 5.

### 2.1. Contents of the UKNDL

The UKNDL comprises data for most of the materials normally needed for reactor physics calculations. The library is subdivided into five files the contents of which can be outlined as follows:

File 1:  $U^{235}$ ,  $U^{233}$ ,  $Pu^{239}$ ,  $U^{238}$  + the main moderating materials

File 2: The remaining heavy nuclides + the main structural materials + the poison materials B, Cd, and Xe

File 3: Some more rarely used materials, for instance materials of interest in experiments

File 4: Photon cross section data file

File 5: Capture cross sections for 78 fission products.

A data set in the library is identified by its "data file number", DFN. The DFN belongs to a substance (nuclide, natural element, molecule, or



mixture), and different data sets for the same substance are given different DFN's.

## 2.2. Data Representation in the UKNDL

For each substance the library may contain data for a number of reactions. Every reaction is identified by the reaction type number, RTN, which is subdivided into a "General classification number", GCN, and a "Particular classification number", PCN. The general classification numbers of interest here are the following:

- 1: Neutron cross section
- 2: Angular distribution of secondary neutrons
- 3: Energy distribution of secondary neutrons
- 4:  $\bar{\nu}$  = mean number of secondary neutrons per fission
- 7: Thermal neutron scattering law data.

The PCN's used in the present library are given in table 2. The reaction type number of a given reaction is formed by combining the GCN and the PCN as follows:

$$RTN = 1000 \times GCN + PCN$$

Example: Angular distribution of neutrons from a (n, 2n) reaction has RTN 2016.

Data with GCN's 1 or 4 (cross sections,  $\bar{\nu}$ ) are tabulated pointwise as a function of energy, the tables consisting of pairs of corresponding values of energy (MeV) and cross sections (barns) or  $\bar{\nu}$ . The energy points are spaced closely enough to ensure that interpolation in a log-log scale will give sufficient accuracy for all energies.

GCN 2 (angular distributions) are given as linear combinations of the probabilities of scattering as a function of  $\cos\theta$ , where  $\theta$  is the scattering angle in either the centre of mass or the laboratory system. Linear interpolation is used between the  $\cos\theta$ -values. Angular distributions may be specified for either energy points or energy ranges. If pointwise representation is used, the distributions for energies in between the points are obtained by linear interpolation.

Energy distributions of secondary neutrons, GCN 3, are specified in the form of energy laws. The laws most often used are:

Table 2

List of PCN's used in the UKNDL, version 1968

1	Total
2	Elastic
3	Non-elastic = total minus elastic
4	(n,n') = total inelastic scattering summed over all final states
5-14	(n,n') to different levels
15	(n,n') to continuum
16	(n, 2n)
17	(n, 3n)
18	fission
22	(n,n') $\alpha$
23	(n,n') $3\alpha$
24	(n, 2n) $\alpha$
25	(n, 3n) $\alpha$
26	(n, 2n) isomeric state
31-50	(n,n') to different levels
101	total parasitic absorption (no secondary neutrons)
102	(n, $\gamma$ )
103	(n, p)
104	(n, d)
105	(n, t)
106	(n, $\text{He}^3$ )
107	(n, $\alpha$ )
108	(n, $2\alpha$ )

- (1) neutrons emitted with energy  $k(E_0 - E_d)$ , where  $k$  is a constant,  $E_0$  the initial energy, and  $E_d$  a constant energy (corresponding to inelastic scattering to a discrete level),
- (2) pointwise tabulated spectrum of secondary neutron energies  $p(E) = f(E)$  independent of initial neutron energy (used for instance for fission spectra),
- (3) or dependent on initial energy  $E_0$  according to the formula  $p\left(\frac{E}{E_0}\right) = f\left(E_0, \frac{E}{E_0}\right)$ , where  $q$  may be 0,  $\frac{1}{2}$ , or 1.

In the case of tabulated probability distributions linear interpolation is used between the points.

Thermal scattering, GCN 7, is in the present version of the UKNDL only available for one material, C, and is therefore not included in the processing code SIGMA.

The data formats are described in more detail in ref. 4.

### 2.3. Use of Library Tapes on the B6700

At the Borroughs B6700 installation of Risø the following UKNDL files with corresponding file names are available:

File 1: AEK 105

File 2: AEK 122

File 3: AEK 121

File 5: AEK 120

The data are filed in EBCDIC card images on 9-track tapes, 800 BPI. The files are written with the file attributes  $KIND = 14$ ,  $MAXRECSIZE = 14$ ,  $BLOCKSIZE = 280$ . A list of the materials and processes on the four files is given in Appendix III.

## 3. THE SIGMA PROCESSING PROGRAM

The processing program SIGMA generates spectrum-averaged multi-group cross sections and transfer matrices from the pointwise tabulated data on the UKNDL. SIGMA is written in ILLINOIS-ALGOL for the IBM7094 machine, but has recently been transferred to the Borroughs B6700. The program is as yet only described in a preliminary internal report<sup>(6)</sup>, but is very similar to the UK program GALAXY<sup>(7)</sup>. The function of SIGMA will be briefly described in the following.

### 3.1. Input Needed for a SIGMA Calculation

SIGMA uses as input the UKNDL file containing data for the materials to be processed. The user specifies the materials and the PCN's for each material and also provides the energy group structure to be used. The spectrum or weighting function over which the cross sections are to be averaged must be given as input, and it may be one of or a linear combination of four standard weighting functions:

- (1)  $F(E) = E^{-x}$  where  $x$  is a constant. If  $x = 1$ , this weighting function corresponds to the  $1/E$ -flux.
- (2)  $F(E) = \frac{1}{(kT)^2} E \cdot \exp(-E/kT)$ . This is the Maxwell spectrum, the value of  $kT$  must be specified.
- (3)  $F(E) = \frac{1}{E[1 + (4.95 \cdot kT/E)^7]}$ . The value of  $kT$  must be specified.

This function is the Westcott delta 2 function, and it may be used to create a smooth joining between the Maxwell and the  $1/E$ -spectrum.

- (4) A tabulated weighting function, given as a number of energy points and corresponding spectrum values. Between the points the program performs log-log interpolation.

### 3.2. Quantities Computed by the Program

For all reactions (PCN's) the program computes the group average cross section in each group:

$$\sigma_g = \frac{\int \sigma(E) F(E) dE}{\int F(E) dE}$$

For all reactions resulting in the formation of secondary neutrons the Legendre moments of the group-to-group transfer matrix will be calculated:

$$\sigma_{g'g}^1 = \frac{1}{\int_g F(E) dE} \int_{g'} dE' \int_g \sigma(E) F(E) dE \int_{-1}^1 P_1(\mu) \Gamma(E, E', \mu) d\mu$$

A is the atomic weight.

This cross section is given PCN 205. It is not to be confused with the transport cross section, PCN 201, described in chapter 4.

Apart from the group cross sections the program calculates a number of material-independent quantities, i. e. quantities only dependent on the group structure and weighting spectrum used. These quantities are:

Group widths in energy

Group widths in lethargy

Group fluxes or normalizing factors,  $\int_g F(E) dE$

Mean reciprocal velocities,  $\frac{\int_g \frac{1}{v} F(E) dE}{\int_g F(E) dE}$

Mean energies,  $\frac{\int_g E F(E) dE}{\int_g F(E) dE}$

Energy corresponding to the mean lethargy,  $\exp\left(\frac{\int_g \ln E F(E) dE}{\int_g F(E) dE}\right)$

Proportion of the standard fission spectrum falling within the groups,

$$0.4527 \int_g \exp\left(-\frac{E}{0.965}\right) \sinh \sqrt{2.29 E} dE$$

An outprint of the material-independent quantities (except the energy widths) calculated by SIGMA is shown in Appendix I.

SIGMA cannot handle all sorts of tabulated information which may be given in the UK-format. Thermal scattering, GCN 7, is not programmed into SIGMA, so when upscattering is important, the data must be supplied from other sources. In the UK-format options exist for tabulating of resolved and unresolved resonance parameters, but in the present version no

tables of this kind are found, and SIGMA cannot process them. GCN 3, energy distributions of secondary neutrons, may be given with a number of energy laws specified; two of them, laws 7 and 10, are not included in SIGMA. Law 7 (ref. 4) is not found in the 1968 version of the UKNDL, law 10 (ref. 3), however, is used once in DFN 328, tantalum.

#### 4. STANDARD COMBINATION

For each material the UKNDL contains data for a number of reactions, characterized by the PCN's mentioned in section 2.2. A SIGMA run for a given material therefore produces cross sections and the required number of scattering matrices for, in some cases, a very great number of reactions. This is not desirable for practical use as neutronics codes normally do not distinguish between, for instance, elastic scattering and inelastic scattering to different levels. The Legendre expansion of scattering matrices will only be utilized in special programs as transport codes used for reference calculations, and most of the everyday codes can only account for scattering anisotropy by a transport correction to the cross sections. So it was decided to edit the group cross sections on the SIGMA MASTER TAPE in a standard combination which is supposed to be convenient for most of the applications.

The standard combination gives for each material the following combined cross sections with corresponding PCN's:

- PCN 502, scattering cross section  
+ transport-corrected scattering matrix
- PCN 101, capture cross section
- PCN 518, fission cross section  
+ fission matrix
- PCN 201, transport cross section.

The scattering cross section, PCN 502, is the sum of the cross sections for all scattering reactions, i.e. PCN 2, PCN 4 or PCN's 5-15 and PCN's 31-50. The processes  $(n, n')$   $\alpha$  and  $(n, n')$   $3\alpha$ , PCN's 22 and 23, will, if they are met for a material, be added to the scattering cross section. The scattering matrix is transport-corrected, whereas the cross section is the total scattering cross section without any correction. The reason for this is that it allows the user of the data to calculate the magnitude of the employed

transport correction by subtracting the sum of the matrix columns from the group cross sections.

The capture cross section, PCN 101, is, if a total parasitic absorption cross section is given for a material, merely the group-averaged cross section for this process, PCN 101. Otherwise it is calculated as the sum of the cross sections for all processes which do not produce secondary neutrons, i. e. PCN's 102-108.

PCN 518, the fission cross section, comprises in addition to PCN 18, fission, all the processes that produce two or more neutrons, PCN's 16, 17, and 24-26. These neutron-multiplicating processes might have been regarded as a sort of inelastic scattering and added to the scattering cross section, but this would in some codes cause difficulties in conserving neutron balance. Their inclusion in the fission cross section has made it necessary to keep the full transfer matrix instead of representing the production of neutrons in the usual way by a fission spectrum and a mean  $\bar{\nu}\sigma_f$  for each group because their secondary neutrons do not emerge with a spectrum independent of the energy of the primary neutron. The full matrix allows representation of an energy-dependent fission spectrum as well, but this has not been of interest with the present version of the UKNDL.

For use in the great number of neutronics codes which only accept a multiplication cross section  $\bar{\nu}\sigma_f$  and a fission spectrum  $\chi$  it is very easy to split the fission matrix into these two commonly used quantities.  $\bar{\nu}\sigma_f$  in all groups is first obtained by summing the columns of the fission matrix:

$$\bar{\nu}\sigma_f^i = \sum_{j=1}^G FM^{ji}$$

where  $\bar{\nu}\sigma_f^i$  is the cross section in group  $i$ ,  $G$  is the number of groups, and  $FM^{ji}$  is the transfer cross section from group  $i$  to group  $j$ . After that an average fission spectrum is calculated by taking the mean value of the scattering into each group from all other groups. The fraction of the fission spectrum falling in group  $i$  will then be:

$$\chi^i = \frac{1}{G} \sum_j FM^{ij} / \bar{\nu}\sigma_f^j$$

In the usual case, where the main contribution to the fission matrix comes from a real fission process, this will be a good approximation.

The transport cross section, PCN 201, is the total cross section minus the transport correction. The total cross section in each group is found by adding the cross sections for PCN's 502, 101, and 518, and the transport cross section is therefore directly flux-weighted like the other cross sections and not inversely averaged as the transport cross section assigned PCN 205.

The transport correction applied is the usual correction suggested by Honeck (ref. 8). For the elastic scattering transfer matrix it is:

$$\sigma_{tr}^{ij} = \sigma_0^{ij} - \frac{1}{2} \sum_{i=1}^G \sigma_1^{ij}$$

where  $\sigma_0^{ij}$  is the zeroth and  $\sigma_1^{ij}$  is the first Legendre moment of the transfer matrix. This correction leaves the off-diagonal elements and thus the energy transfer characteristics unaltered. The transport cross section in group  $j$  is obtained from the total cross section correspondingly:

$$\sigma_{tr}^j = \sigma_{total}^j - \sum_{i=1}^G \sigma_1^{ij}$$

To the inelastic part of the scattering no correction for anisotropy is made, because the transport correction of Honeck over-corrects the cross sections when neutrons are scattered from high-energy groups directly into groups of low energy. This is discussed in ref. 9.

## 5. GROUP STRUCTURE

It was the intention that the SIGMA MASTER TAPE should be adequate for use on a wide range of reactor types. This means that the energy groups applied must be sufficiently narrow to ensure that the group cross sections will be reasonably independent of the weighting spectrum used in SIGMA. On the other hand the number of energy groups is limited by practical considerations, as it ought to be possible to perform a spectrum calculation for at least a 3-region cell in the MASTER TAPE group structure.

At Rise the previous multi-group library has been that of LASER with its 85-group structure as described in ref. 10. About 85 groups was thought to be a realistic maximum considering the size of available computers. For the sake of continuity the LASER 85-group structure was chosen as the



starting point, and after the introduction of some modifications the result was a structure with 76 groups. These 76 energy groups are shown in Appendix I as an outprint from the SIGMA program.

The thermal energy mesh was taken over directly from LASER. It consists of 35 groups between 0 and 1.855 eV. Above the upper limit of the thermal mesh upscattering is assumed to be negligible. As seen from table 5 the group limits are round numbers in speed units of 2200 m/s which of course implies that the corresponding group energy boundaries and the lethargy widths have rather awkward values. A number of very narrow groups are placed around the  $\text{Pu}^{240}$  resonance at 1.0 eV, and the  $\text{Pu}^{239}$  resonance at 0.3 eV is treated similarly, but it is given fewer groups as it is low and broad compared with the sharp resonance of  $\text{Pu}^{240}$ . By means of these narrow groups the self-shielding of the two resonances is supposed to be accounted for, at least approximately, during Pu build-up, so that one set of microscopic group cross sections may be used for all geometries throughout depletion.

Apart from the two concentrations around the resonances, the thermal energy mesh is nearly equidistant in lethargy from about 0.05 eV and upwards where the thermal flux peak of an undermoderated light-water reactor is situated; downwards the groups get broader.

The fast and epithermal energy mesh of LASER is the well-known MUFT mesh starting from 10 MeV and stepping down in 0.25 lethargy unit steps until 67 keV. From here until 0.167 keV the lethargy widths are 0.5, and the rest of the way down to the thermal mesh it is again 0.25.

The fast part of the MUFT group structure is kept unaltered apart from one extra group which is added from 10 to 15 MeV. The reason for this is that the UKNDL contains data for energies up to 15 MeV.

In the resonance energy region it is of no use to try to make the groups narrow enough to represent the strongly energy-varying cross sections adequately. This would require thousands of groups. Instead one has to calculate the resonance broad group cross sections separately for each case, and they will be dependent both on geometry and on temperature. It is, however, possible to facilitate the resonance calculation by proper selection of the group boundaries.

First of all care should be taken to ensure that no important resonance is cut in two by a group boundary. But if the resonances in a group are either many uniformly distributed or one single resonance situated near the lethargy midpoint, it is in addition true to a good approximation that the group absorption cross section is independent of the source depletion through

Table 5

LASER thermal energy mesh

i	Speed <sup>a</sup>	Mesh width <sup>a</sup>	Energy	E <sub>int</sub> (ev)
	v <sub>i</sub>	Δ v <sub>i</sub>	E <sub>i</sub> (ev)	
1	.2	.2	.001012	.002277
2	.4	.2	.004048	.006325
3	.6	.2	.009108	.012397
4	.8	.2	.016192	.020493
5	1.0	.2	.0253	.030613
6	1.2	.2	.036432	.042757
7	1.4	.2	.049588	.056925
8	1.65	.3	.068879	.081972
9	1.95	.3	.096203	.11157
10	2.25	.3	.12808	.14573
11	2.55	.3	.16451	.18444
12	2.85	.3	.20550	.22770
13	3.075	.15	.23923	.25104
14	3.21	.12	.26069	.27053
15	3.33	.12	.28055	.29075
16	3.42	.06	.29592	.30113
17	3.505	.11	.31081	.32064
18	3.66	.2	.33891	.35768
19	3.91	.3	.38679	.41704
20	4.26	.4	.45913	.50326
21	4.715	.51	.56245	.62493
22	5.265	.59	.70132	.78211
23	5.845	.57	.86435	.95070
24	6.23	.2	.98197	1.01374
25	6.375	.09	1.02821	1.04277
26	6.435	.03	1.04765	1.05254
27	6.465	.03	1.05744	1.06236
28	6.495	.03	1.06728	1.07222
29	6.55	.08	1.08543	1.09873
30	6.69	.2	1.13233	1.16645
31	6.99	.4	1.23616	1.30791
32	7.39	.4	1.38169	1.45748
33	7.765	.35	1.52547	1.59500
34	8.10	.32	1.65993	1.72616
35	8.41135	.3027	1.79000	1.85500

<sup>a</sup>

1 unit = 2200 m/s

the group as shown by Askew in ref. 11. This will make it possible to calculate the resonance group cross sections on the basis of one single tabulation for each material.

In the LASER energy structure some of the group boundaries lie very close to important resonances. For that reason a number of group boundaries have been removed in the energy region from 1.855 eV up to 200 eV so that 18 groups are collapsed into only 8 groups. The main single resonances became situated near the middle of the lethargy interval of these broad groups.

In fig. 5 a, b, and c the resulting 76-group structure is shown. The original LASER structure is shown too for comparison. A light-water reactor spectrum was drawn to illustrate how the groups are concentrated round the fission spectrum at high energies and at the thermal part of the spectrum where also the two concentrations of very narrow groups are situated. In addition the energies of the low-lying  $U^{238}$  resonances are marked.

Although this group structure was designed mainly with reference to light-water reactors, it is hoped that it will be adequate for other reactor types as well. The 69-group structure used in WIMS (ref. 12) and in FLEF (ref. 13) is constructed according to similar principles and has been in use for both heavy-water- and graphite-moderated reactors. A group set commonly used for calculations on fast systems, the Bondarenko set (ref. 14), is included in fig. 5 showing that the fast part of the Rissø 76-group system will presumably be suitable for fast reactor calculations.

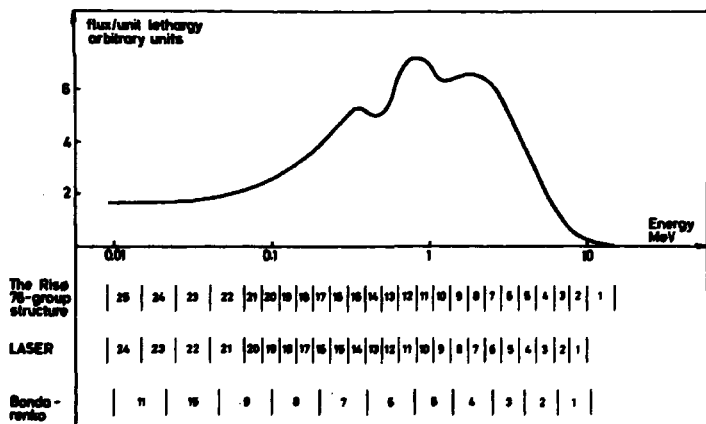


Fig 5a. Energy groups. Fast part.

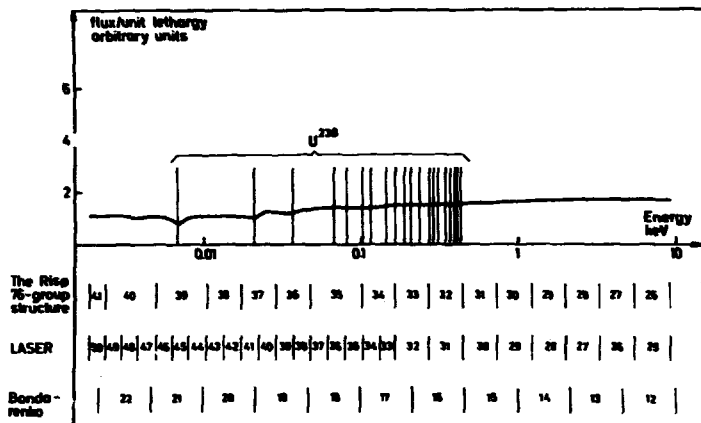


Fig. 5b. Energy groups. Intermediate part.

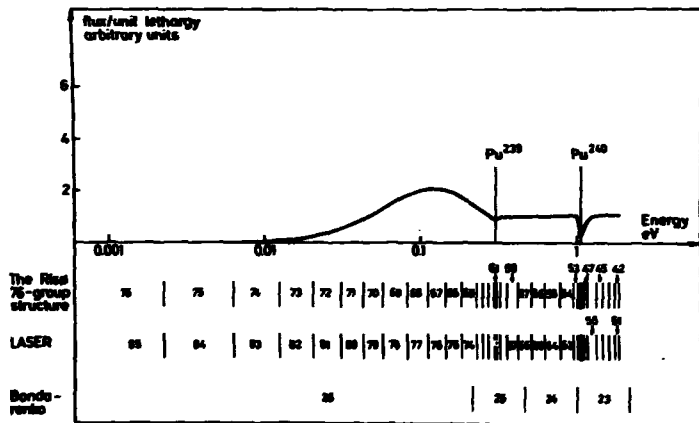


Fig. 5c. Energy groups. Thermal part.

## 6. WEIGHTING FUNCTION

Before the weighting function to be used for the SIGMA MASTER TAPE was chosen, a number of test runs were made where different weighting functions were used to generate cross sections for a number of materials in the 76-group structure decided upon. In resonance regions the group cross sections of course proved to be very spectrum-dependent, but where no resonances were present the most diverging weighting spectra gave a difference in the group cross section of only a few per cent. The conclusion drawn from this is that the groups of the 76-group structure are sufficiently narrow for a cross section tape intended for use on reactors with differing spectra.

As the weighting function seemed to be rather uncritical as long as it was not strongly inclined to the wrong side, a very simple combination of the standard weight functions available in SIGMA was chosen for the SIGMA MASTER TAPE. At low energies a Maxwell spectrum was used:

$$F(E) = \frac{1}{(kT)^2} E \cdot \exp \left( - \frac{E}{kT} \right)$$

with

$$kT = 0.05 \text{ eV}$$

For all other energies the weighting function is simply

$$F(E) = \frac{1}{E}$$

The change from Maxwell to  $\frac{1}{E}$  weighting was put between groups Nos. 63 and 64, i. e. at the energy 0.25 eV.

In resonance regions this weighting yields group cross sections for infinite dilution at the UKNDL temperature which is 300 degrees absolute.

## 7. UTILIZATION OF THE MASTER TAPE DATA IN THE PROGRAM SYSTEM AT RISØ

The SIGMA MASTER TAPE is one link in an attempt to build up a data generating system which produces constants for reactor physics calculations on the basis of fundamental nuclear data exclusively. Before the group cross sections are used in neutronics programs, they have to be supplied with thermal scattering data if the system in question is a thermal one, and with shielded resonance cross sections whenever the resonance absorbers may not be considered as infinitely dilute. This combination is performed in a program called CRS. After the cross sections for a given reactor configuration have been prepared, the code can make a spectrum calculation, collapse the cross sections into fewer groups, and punch the collapsed cross sections out in formats corresponding to the input requirements for a number of codes.

The thermal transfer cross sections are at present produced by a routine, NELKINSCM, which is incorporated in CRS. NELKINSCM (ref. 15) calculates thermal scattering matrices for H bound in  $H_2O$  and D in  $D_2O$  on the basis of the NELKIN model for H and the similar model for D. All other materials are treated as perfectly gaseous. In the near future this direct calculation of thermal scattering matrices is to be replaced by a thermal "master tape", where the transfer matrices will be filed for relevant materials at a number of temperatures close enough to allow linear interpolation between group cross sections in temperature. By the introduction of these tabulations much computer time will be saved, and at the same time the accuracy of the cross sections will be better as it is of course possible in the preparation of such tables to use more sophisticated methods than in a calculation which has to be made for every single case.

Effective resonance cross sections are introduced for  $U^{238}$  in 22 groups and for  $U^{235}$  and  $Pu^{239}$  in 14 groups. In both cases the lowest resonance group is the one just above the thermal upper limit, which means that the resonance region is defined to be 1.855 eV - 111 keV for  $U^{238}$  and 1.855 eV - 3.35 keV for  $U^{235}$  and  $Pu^{239}$ . The resonance cross sections may be calculated by the RESAB PROGRAM SYSTEM (refs. 16 and 17) or in the CRS program itself by the routine RESOREX (ref. 18) which generates resonance group cross sections by means of an equivalence principle on the basis of tabulations from RESAB. For all other resonant materials the dilute cross sections from the SIGMA MASTER TAPE are normally kept unaltered. In cases where shielding effects are considered important, the cross sections

may, however, be calculated by RESAB and substituted into the data set by hand.

For burn-up calculations a 10-energy group subsystem of the 76 MASTER TAPE groups is normally used in the burn-up codes CEB and CDB (ref. 19) in current use at Risø. As the 76-group spectrum changes because of build-up of Pu and fission products, it is advisable to regenerate the 10-group cross sections with revised isotopic composition at intervals during burn-up. If RESOREX is used, it is furthermore important to generate the  $\text{Pu}^{239}$  cross sections for a composition where a reasonable amount of  $\text{Pu}^{239}$  is present as demonstrated in ref. 18.

Frequent alternation between spectrum calculation in 76 groups and burn-up in 10 groups is possible for a pin cell burn-up calculation by the CEB program, but unrealistic in a box code like CDB. Fortunately it seems that 10-group cross sections generated by a spectrum calculated a few time steps from start may be used all through the burn-up calculation, giving an accuracy which is quite sufficient for most purposes.

## 8. CONTENTS OF THE CROSS SECTION LIBRARY

In its present version the SIGMA MASTER TAPE contains 126 materials which are almost all those available from the UKNDL, version 1968. For some materials only cross sections for a special reaction and in some cases for a limited energy range are given - these tables are not considered well suited for the standard combination described in chapter 4 and are therefore omitted. A single material was omitted because the SIGMA program at present cannot handle law number 10 for energy distribution of secondary neutrons which is used only in the tabulation for tatalum, DFN 328.

Each material on the SIGMA MASTER TAPE has an identification number which is to be used for seeking out the material. These numbers are written in order in one of the first records of the tape.

The cross sections are given in the standard combination which is described in chapter 4. In the combination all relevant detailed processes tabulated for each material are included. The UKNDL specifies data for detailed reactions by means of particular classification numbers, PCN's, as described in section 2.2. In Appendix III a listing is given of the reactions of the different materials.

### 8.1. Table of the Contents

In table 8.1 the SIGMA MASTER TAPE contents are listed. The materials are put in order of increasing mass number apart from the 78 fission products from UKNDL file 5 which are taken last. For each material the identification number is given, and the processes from the standard combination that are found for a particular material are given.

For most substances only one file on the UKNDL is available. In cases of doubt it is noted in the table which DFN has been used. Where an element is mentioned without mass number, the cross section set refers to the natural isotopic composition.

The pseudo-fission-product called FP is generated from DFN 106 in the UKNDL. Since no information is given about the reactor configuration to which it applies, great care should be taken in using it for reactor physics calculations. The large absorption cross section indicates that all fission products are included, i. e. also Xe and Sm.

### 8.2. Sequence of Materials

To minimize the computer time wasted on the reading of the magnetic tape, care was taken to place the materials so that those most often used are set first. In table 8.2 the materials are listed in the same sequence as on the tape.

### 8.3. Missing Materials and Energy Regions

A number of materials of interest in reactor physics calculations are not included in the UKNDL and are consequently not found on the SIGMA MASTER TAPE either. Such materials must, when necessary, be taken from other sources. For example  $\text{Pu}^{242}$ , Ag, and In are missing.

In some cases the cross sections of the UKNDL are only tabulated for a smaller energy range than the standard range from  $10^{-4}$  eV to 15 MeV. In energy groups where no data exist the cross sections are set equal to zero, and the limited energy range is noted in table 8.1. For some of the materials, however, the data stop at 10 MeV so that the cross section in the first energy group is zero. This has not caused any comment in the table.



Table 8. 1

Contents of the SIGMA MASTER TAPE

Material	Number	PCN's				Comments
		502 + matrix	101	518 + matrix	201	
H	41	x	x		x	
H <sub>2</sub> O	34	x	x		x	Only for energies < 0.5 eV
D	42	x	x	x	x	
D <sub>2</sub> O	33	x	x		x	Only for energies < 9 eV
T	61	x	x	x	x	
He <sup>3</sup>	66	x	x		x	Temperature 0 K
He <sup>4</sup>	67	x	x		x	Temperature 0 K
Li <sup>6</sup>	68	x	x	x	x	
Li <sup>7</sup>	69	x	x	x	x	Temperature 0 K
Be <sup>9</sup>	40	x	x	x	x	
B	50	x	x		x	
B <sup>10</sup>	64	x	x		x	
B <sup>11</sup>	65	x	x		x	
C	32	x	x		x	
N	71	x	x	x	x	
O	31	x	x		x	DFN 34 has been used
F	70	x	x	x	x	
Na	46	x	x	x	x	DFN 182 has been used
Al	35	x	x	x	x	DFN 35 has been used
Si	63	x	x		x	
Cl	73	x	x	x	x	
Ca	72	x	x		x	
Ti	75	x	x	x	x	
Cr	38	x	x	x	x	
Mn <sup>55</sup>	51		x			
Fe	37	x	x		x	
Ni	39	x	x	x	x	
Cu	53	x	x	x	x	
Ga	74	x	x	x	x	

Material	Number	PCN's				Comments
		502 + matrix	101	518 + matrix	201	
Zr	36	x	x	x	x	
Cd	49	x	x	x	x	
Xe <sup>135</sup>	19	x	x		x	
Sm <sup>149</sup>	15		x			Identical with fission product No. 767
Gd	76		x			Only for energies <3 eV
W	57	x	x	x	x	
Au <sup>197</sup>	58	x	x	x	x	
Pb	43	x	x	x	x	
Th <sup>232</sup>	1	x	x	x	x	
U <sup>233</sup>	3	x	x	x	x	
U <sup>234</sup>	4	x	x	x	x	Only for energies >1 keV
U <sup>235</sup>	5	x	x	x	x	
U <sup>236</sup>	6	x	x	x	x	Only for energies >1 keV
U <sup>238</sup>	7	x	x	x	x	
Pu <sup>238</sup>	62	x	x	x	x	
Pu <sup>239</sup>	9	x	x	x	x	
Pu <sup>240</sup>	10	x	x	x	x	
Pu <sup>241</sup>	11	x	x	x	x	
FP	28	x	x	x	x	Pseudo-fission- products
Br <sup>81</sup>	701		x			
Se <sup>82</sup>	702		x			
Kr <sup>83</sup>	703		x			
Kr <sup>84</sup>	704		x			
Kr <sup>85</sup>	705		x			
Rb <sup>85</sup>	706		x			
Kr <sup>86</sup>	707		x			
Rb <sup>87</sup>	708		x			
Sr <sup>88</sup>	709		x			
Sr <sup>89</sup>	710		x			
Y <sup>89</sup>	711		x			

Material	Number	PCN's				Comments
		502 + matrix	101	518 + matrix	201	
Sr <sup>90</sup>	712		x			
Y <sup>90</sup>	713		x			
Y <sup>91</sup>	714		x			
Zr <sup>91</sup>	715		x			
Zr <sup>92</sup>	716		x			
Zr <sup>93</sup>	717		x			
Zr <sup>94</sup>	718		x			
Mo <sup>95</sup>	719		x			
Zr <sup>96</sup>	720		x			
Mo <sup>97</sup>	721		x			
Mo <sup>98</sup>	722		x			
Tc <sup>99</sup>	723		x			
Mo <sup>100</sup>	724		x			
Ru <sup>101</sup>	725		x			
Ru <sup>102</sup>	726		x			
Rh <sup>103</sup>	727		x			
Ru <sup>104</sup>	728		x			
Rh <sup>105</sup>	729		x			
Pd <sup>105</sup>	730		x			
Pd <sup>106</sup>	731		x			
Pd <sup>107</sup>	732		x			
Pd <sup>108</sup>	733		x			
Ag <sup>109</sup>	734		x			
Cd <sup>113</sup>	735		x			
In <sup>115</sup>	736		x			
Sb <sup>125</sup>	737		x			
I <sup>127</sup>	738		x			
Te <sup>128</sup>	739		x			
I <sup>129</sup>	740		x			
Te <sup>130</sup>	741		x			
I <sup>131</sup>	742		x			
Xe <sup>131</sup>	743		x			
Xe <sup>132</sup>	744		x			
Xe <sup>133</sup>	745		x			
Cs <sup>133</sup>	746		x			

Material	Number	PCN's				Comments
		502 + matrix	101	518 + matrix	201	
Xe <sup>134</sup>	747		x			
Cs <sup>134</sup>	748		x			
I <sup>135</sup>	749		x			
Xe <sup>135</sup>	750		x			
Cs <sup>135</sup>	751		x			
Xe <sup>136</sup>	752		x			
Cs <sup>137</sup>	753		x			
Ba <sup>138</sup>	754		x			
La <sup>139</sup>	755		x			
Ce <sup>140</sup>	756		x			
Pr <sup>141</sup>	757		x			
Ce <sup>142</sup>	758		x			
Nd <sup>143</sup>	759		x			
Nd <sup>144</sup>	760		x			
Nd <sup>145</sup>	761		x			
Nd <sup>146</sup>	762		x			
Pm <sup>147</sup>	763		x			
Nd <sup>148</sup>	764		x			
Pm <sup>148</sup>	765		x			
Pm <sup>148m</sup>	766		x			
Sm <sup>148</sup>	767		x			
Nd <sup>150</sup>	768		x			
Sm <sup>150</sup>	769		x			
Sm <sup>151</sup>	770		x			
Sm <sup>152</sup>	771		x			
Eu <sup>153</sup>	772		x			
Sm <sup>154</sup>	773		x			
Eu <sup>154</sup>	774		x			
Eu <sup>155</sup>	775		x			
Gd <sup>155</sup>	776		x			
Gd <sup>156</sup>	777		x			
Gd <sup>157</sup>	778		x			

Table 8.2

Materials in order as filed on the tape

No.	Identification number	Material	No.	Identification number	Material
1	5	U <sup>235</sup>	35	63	Si
2	7	U <sup>238</sup>	36	64	B <sup>10</sup>
3	41	H	37	65	B <sup>11</sup>
4	42	D	38	66	He <sup>3</sup>
5	31	O	39	67	He <sup>4</sup>
6	32	C	40	68	Li <sup>6</sup>
7	34	H <sub>2</sub> O	41	69	Li <sup>7</sup>
8	33	D <sub>2</sub> O	42	70	F
9	40	Be <sup>9</sup>	43	71	N
10	46	Na	44	72	Ca
11	36	Zr	45	73	Cl
12	37	Fe	46	74	Ga
13	38	Cr	47	75	Ti
14	39	Ni	48	76	Gd
15	35	Al	49	701	Br <sup>81</sup>
16	50	B	50	702	Se <sup>82</sup>
17	49	Cd	51	703	Kr <sup>83</sup>
18	9	Pu <sup>239</sup>	52	704	Kr <sup>84</sup>
19	10	Pu <sup>240</sup>	53	705	Kr <sup>85</sup>
20	11	Pu <sup>241</sup>	54	706	Rb <sup>85</sup>
21	6	U <sup>236</sup>	55	707	Kr <sup>86</sup>
22	1	Th <sup>232</sup>	56	708	Rb <sup>87</sup>
23	3	U <sup>233</sup>	57	709	Sr <sup>88</sup>
24	4	U <sup>234</sup>	58	710	Sr <sup>89</sup>
25	19	Xe <sup>135</sup>	59	711	Y <sup>89</sup>
26	28	FP	60	712	Sr <sup>90</sup>
27	15	Sm <sup>149</sup>	61	713	Y <sup>90</sup>
28	53	Cu	62	714	Y <sup>91</sup>
29	58	Au <sup>197</sup>	63	715	Zr <sup>91</sup>
30	57	W	64	716	Zr <sup>92</sup>
31	43	Pb	65	717	Zr <sup>93</sup>
32	51	Mn <sup>55</sup>	66	718	Zr <sup>94</sup>
33	61	T	67	719	Mo <sup>95</sup>
34	62	Pu <sup>238</sup>	68	720	Zr <sup>96</sup>

No.	Identification number	Material
69	721	Mo <sup>97</sup>
70	722	Mo <sup>98</sup>
71	723	Tc <sup>99</sup>
72	724	Mo <sup>100</sup>
73	725	Ru <sup>101</sup>
74	726	Ru <sup>102</sup>
75	727	Rh <sup>103</sup>
76	728	Ru <sup>104</sup>
77	729	Rh <sup>105</sup>
78	730	Pd <sup>105</sup>
79	731	Pd <sup>106</sup>
80	732	Pd <sup>107</sup>
81	733	Pd <sup>108</sup>
82	734	Ag <sup>109</sup>
83	735	Cd <sup>113</sup>
84	736	In <sup>115</sup>
85	737	Sb <sup>125</sup>
86	738	I <sup>127</sup>
87	739	Te <sup>128</sup>
88	740	I <sup>129</sup>
89	741	Te <sup>130</sup>
90	742	I <sup>131</sup>
91	743	Xe <sup>131</sup>
92	744	Xe <sup>132</sup>
93	745	Xe <sup>133</sup>
94	746	Cs <sup>133</sup>
95	747	Xe <sup>134</sup>
96	748	Cs <sup>134</sup>
97	749	I <sup>135</sup>
98	750	Xe <sup>135</sup>
99	751	Cs <sup>135</sup>
100	752	Xe <sup>136</sup>
101	753	Cs <sup>137</sup>
102	754	Ba <sup>138</sup>
103	755	La <sup>139</sup>

No.	Identification number	Material
104	756	Ce <sup>140</sup>
105	757	Pr <sup>141</sup>
106	758	Ce <sup>142</sup>
107	759	Nd <sup>143</sup>
108	760	Nd <sup>144</sup>
109	761	Nd <sup>145</sup>
110	762	Nd <sup>146</sup>
111	763	Pm <sup>147</sup>
112	764	Nd <sup>148</sup>
113	765	Pm <sup>148</sup>
114	766	Pm <sup>148m</sup>
115	767	Sm <sup>149</sup>
116	768	Nd <sup>150</sup>
117	769	Sm <sup>150</sup>
118	770	Sm <sup>151</sup>
119	771	Sm <sup>152</sup>
120	772	Eu <sup>153</sup>
121	773	Sm <sup>154</sup>
122	774	Eu <sup>154</sup>
123	775	Eu <sup>155</sup>
124	776	Gd <sup>155</sup>
125	777	Gd <sup>156</sup>
126	778	Gd <sup>157</sup>

## 9. MAGNETIC TAPE STRUCTURE

### 9.1. Format of the Binary Tape

In deciding upon the format of the binary tape the philosophy was that of making the tape easy to read by user programs rather than that of saving magnetic tape space. One result of this is that the full scattering matrices were recorded, although in some cases they mostly consist of noughts.

In the following the contents of the binary tape are listed record by record. All arrays running over energy groups start in group 1 which is the group of highest energy.

#### (a) 4 Words:

- |              |   |
|--------------|---|
| SET, integer | = set number of the data on the tape, refers to the group structure and weighting function used. The present version has set number 1 |
| GRP, integer | = number of energy groups   |
| MAT, integer | = number of materials   |
| LEG, integer | = maximal order of Legendre moments for scattering matrices which is 0 for the standard combination used on the SIGMA MASTER TAPE     |

#### (b) 8 x GRP + MAT + 1 Words (nine physical records, one for each array):

- |                              |   |
|------------------------------|---|
| E [0:GRP], real array        | = energy group boundaries (MeV)                                       |
| DE [1:GRP], real array       | = group energy widths (MeV)   |
| DU [1:GRP], real array       | = group lethargy widths   |
| NORM [1:GRP], real array     | = group normalizing factors   |
| EMEAN [1:GRP], real array    | = weighted group mean energies (MeV)                                  |
| EUMEAN [1:GRP], real array   | = energies corresponding to the weighted group mean lethargies (MeV)  |
| VRECMEAN [1:GRP], real array | = group mean reciprocal velocities (s/cm)                             |
| FISP [1:GRP], real array     | = fraction of the standard fission spectrum falling within each group |
| NUMB [1:MAT], integer array  | = identification numbers of the materials on the tape                 |

The following is repeated for all materials, i. e. MAT times

(c) 6 Words:

DFN, integer = data file number from the UKNDL for the material  
AW, real = atomic weight (amu)  
Z, integer = atomic number  
TXT = alphanumeric name of the material (6 characters)  
NPCA, integer = number of PCN's given for this material (NPCA is 1, 3, or 4 on the SIGMA MASTER TAPE)  
N, integer = identification number of the material. This number is one of the elements of the NUMB array in record b.

(d) 2 x NPCA Words:

PCN [1:NPCA], integer array = particular classification numbers for the NPCA different cross section types of the material  
MIND [1:NPCA], integer array = matrix indicators. An element of the MIND array is 1 if the corresponding cross section is followed by a scattering matrix, if not, it is -1.

The following records, type e and, if the MIND-element is 1, GRP times type f, are repeated NPCA times, i. e. once for each cross section type of the material.

(e) GRP Words:

SIG [1:GRP], real array = group cross sections

(f) GRP Words:

SM [I, 1:GRP], real array = transfer cross section to group I from all other groups

Record f is repeated GRP times, I running from 1 to GRP, to give the full scattering matrix.

After the last material an END-OF-FILE mark is written.



## 9.2. Characteristics of the Tape Version for Use on the B6700

The SIGMA MASTER TAPE in use on the Borroughs B6700 computer at Risø is a 9-track 800 BPI binary tape. It is written with the file attribute FILETYPE = 0 which means constant physical record length equal to the value of the file attribute MAXRECSIZE. The records are unblocked. Two versions of the SIGMA MASTER TAPE exist at present:

A 2400-feet tape labelled AEK134 containing all 126 materials. This version is filed with MAXRECSIZE = 126.

A 1200-feet tape labelled AEK42 which contains only the first 32 materials. It has MAXRECSIZE = 77.

In case the binary tape is spoiled, for instance by a parity error, it may be regenerated from a card image version by use of a small program called MTBIN. This is described in Appendix II.

## ACKNOWLEDGEMENTS

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## APPENDIX I

### OUTPRINT OF THE GROUP STRUCTURE FROM THE SIGMA PROGRAM

On the following pages the 76-group structure is shown as printed out by the SIGMA program. Apart from the energy boundaries the group structure is characterized by the lethargy widths of the groups and by the proportion of the standard fission spectrum belonging to each group (section 3.2). The quantities average energy, energy at average lethargy, and average inverse velocity are dependent on the weighting function specified, in this case the weighting function used for the SIGMA MASTER TAPE as described in chapter 6. The group constants called NORM in the table are the group fluxes, i. e. the weighting function integrated for each group.

GROUP NUMBER	ENERGY BOUNDARIES (MEV)	AVERAGE ENERGY (MEV)	ENERGY AT AVERAGE LETARASY (MEV)	LETARASY HIGH	FRACTION OF STANDARD FISSION SPECTRUM	AVERAGE INVERSE VELOCITY (1/VELOC)	NOTE
1.	1.5000E-01	1.2330E-01	1.2247E-01	4.0547E-01	0.00360	2.0697E-08	4.3547E-01
2.	1.0000E-01	4.0400E-00	8.0250E-00	2.5000E-01	0.00511	2.4396E-08	2.5000E-01
3.	7.7000E-00	6.0000E-00	6.8729E-00	2.5000E-01	0.01705	2.7599E-08	2.5000E-01
4.	4.0653E-00	5.3666E-00	5.3526E-00	2.5000E-01	0.03944	3.1274E-08	2.5000E-01
5.	4.7237E-00	4.1795E-00	4.1686E-00	2.5000E-01	0.06872	3.5438E-08	2.5000E-01
6.	3.6790E-00	3.2550E-00	3.2465E-00	2.5000E-01	0.09625	4.0196E-08	2.5000E-01
7.	2.6490E-00	2.5550E-00	2.5254E-00	2.5000E-01	0.11403	4.5503E-08	2.5000E-01
8.	2.2313E-00	1.9742E-00	1.9691E-00	2.5000E-01	0.11805	5.1962E-08	2.5000E-01
9.	1.7377E-00	1.5379E-00	1.5335E-00	2.5000E-01	0.11236	5.8627E-08	2.5000E-01
10.	1.3533E-00	1.1974E-00	1.1945E-00	2.5000E-01	0.09059	6.6207E-08	2.5000E-01
11.	1.0540E-00	9.3257E-01	9.3014E-01	2.5000E-01	0.08174	7.5027E-08	2.5000E-01
12.	8.2095E-01	7.2629E-01	7.2442E-01	2.5000E-01	0.06489	8.5011E-08	2.5000E-01
13.	6.3920E-01	5.6563E-01	5.6416E-01	2.5000E-01	0.04984	9.6530E-08	2.5000E-01
14.	4.9787E-01	4.4051E-01	4.3937E-01	2.5000E-01	0.03732	1.0916E-07	2.5000E-01
15.	3.8774E-01	3.4507E-01	3.4218E-01	2.5000E-01	0.02741	1.2349E-07	2.5000E-01
16.	3.0297E-01	2.6719E-01	2.6449E-01	2.5000E-01	0.01983	1.4016E-07	2.5000E-01
17.	2.3510E-01	2.0000E-01	2.0754E-01	2.5000E-01	0.01418	1.5603E-07	2.5000E-01
18.	1.8316E-01	1.6206E-01	1.6163E-01	2.5000E-01	0.01005	1.7997E-07	2.5000E-01
19.	1.4264E-01	1.2621E-01	1.2588E-01	2.5000E-01	0.00708	2.0393E-07	2.5000E-01
20.	1.1109E-01	9.6292E-02	9.6037E-02	2.5000E-01	0.00495	2.3508E-07	2.5000E-01
21.	8.6517E-02	7.6590E-02	7.6391E-02	2.5000E-01	0.00345	2.6196E-07	2.5000E-01
22.	6.7379E-02	5.3024E-02	5.2475E-02	5.0000E-01	0.00407	3.1647E-07	5.0000E-01
23.	4.0668E-02	3.2160E-02	3.1828E-02	5.0000E-01	0.00195	4.0656E-07	5.0000E-01
24.	2.4787E-02	1.9506E-02	1.9325E-02	5.0000E-01	0.00093	5.2177E-07	5.0000E-01
25.	1.5034E-02	1.1831E-02	1.1709E-02	5.0000E-01	0.00044	5.6997E-07	5.0000E-01
26.	9.1168E-03	7.1759E-03	7.1017E-03	5.0000E-01	0.00021	8.6026E-07	5.0000E-01
27.	5.3308E-03	4.3524E-03	4.3074E-03	5.0000E-01	0.00010	1.1046E-06	5.0000E-01
28.	3.3546E-03	2.6599E-03	2.6126E-03	5.0000E-01	0.00005	1.4182E-06	5.0000E-01
29.	2.0547E-03	1.6012E-03	1.5846E-03	5.0000E-01	0.00002	1.8212E-06	5.0000E-01
30.	1.2341E-03						

30.	7.4092E-04	9.7116E-04	9.6111E-04	5.0000E-01	0.00001	2.5984E-06	5.0000E-01
31.	4.9400E-04	5.8904E-04	5.6295E-04	5.0000E-01	0.00000	3.0006E-06	5.0000E-01
32.	2.7536E-04	3.5727E-04	3.5598E-04	5.0000E-01	0.00000	3.8554E-06	5.0000E-01
33.	2.1669E-04	2.1669E-04	2.1448E-04	5.0000E-01	0.00000	4.0505E-06	5.0000E-01
34.	1.6702E-04	1.3143E-04	1.3007E-04	5.0000E-01	0.00000	4.5569E-06	5.0000E-01
35.	1.0130E-04	7.1266E-05	6.9623E-05	7.0000E-01	0.00000	8.7166E-06	7.5000E-01
36.	4.7851E-05	3.7656E-05	3.7267E-05	5.0000E-01	0.00000	1.1876E-05	5.0000E-01
37.	2.9023E-05	2.2840E-05	2.2603E-05	5.0000E-01	0.00000	1.8240E-05	5.0000E-01
38.	1.7603E-05	1.3853E-05	1.3713E-05	5.0000E-01	0.00000	1.9579E-05	5.0000E-01
39.	1.0677E-05	7.5114E-06	7.5382E-06	7.0000E-01	0.00000	2.6849E-05	7.5000E-01
40.	5.0435E-06	3.5401E-06	3.6663E-06	7.0000E-01	0.00000	3.9669E-05	7.5000E-01
41.	2.3624E-06	2.1077E-06	2.1022E-06	2.5021E-01	0.00000	4.0993E-05	2.5021E-01
42.	1.6590E-06	1.7898E-06	1.7894E-06	7.1962E-02	0.00000	5.4056E-05	7.1962E-02
43.	1.7262E-06	1.6597E-06	1.6593E-06	7.9849E-02	0.00000	5.6137E-05	7.9849E-02
44.	1.9950E-06	1.5232E-06	1.5267E-06	9.0191E-02	0.00000	6.9563E-05	9.0191E-02
45.	1.4573E-06	1.3814E-06	1.3807E-06	1.0838E-01	0.00000	8.1544E-05	1.0838E-01
46.	1.8179E-06	1.2358E-06	1.2391E-06	1.1450E-01	0.00000	6.5071E-05	1.1450E-01
47.	1.1664E-06	1.1322E-06	1.1323E-06	5.9794E-02	0.00000	6.7962E-05	5.9794E-02
48.	1.0907E-06	1.0854E-06	1.0853E-06	2.4415E-02	0.00000	6.9466E-05	2.4415E-02
49.	1.3722E-06	1.0673E-06	1.0674E-06	9.1821E-03	0.00000	8.9991E-05	9.1821E-03
50.	1.0624E-06	1.0574E-06	1.0574E-06	9.3622E-03	0.00000	7.0324E-05	9.3622E-03
51.	1.0525E-06	1.0676E-06	1.0677E-06	9.2589E-03	0.00000	7.0644E-05	9.2589E-03
52.	1.0428E-06	1.0282E-06	1.0281E-06	2.8380E-02	0.00000	7.1311E-05	2.8380E-02
53.	1.0137E-06	9.8186E-07	9.8171E-07	6.4164E-02	0.00000	7.2981E-05	6.4164E-02
54.	9.5070E-07	8.6366E-07	8.6229E-07	1.9525E-01	0.00000	7.7898E-05	1.9525E-01
55.	7.6211E-07	7.0058E-07	6.9912E-07	2.2436E-01	0.00000	5.6523E-05	2.2436E-01
56.	6.2493E-07	5.6198E-07	5.6081E-07	2.1653E-01	0.00000	9.6602E-05	2.1653E-01
57.	5.0326E-07	4.5888E-07	4.5812E-07	1.8792E-01	0.00000	1.0687E-04	1.8792E-01
58.	4.1704E-07	3.8668E-07	3.8622E-07	1.9554E-01	0.00000	1.1630E-04	1.9554E-01
59.	3.5768E-07	3.1882E-07	3.1869E-07	1.3932E-01	0.00000	1.2487E-04	1.3932E-01
60.	3.2046E-07						

60.	3.0113E-07	3.1873E-07	3.1073E-07	6.8777E-02	0.00000	1.8792E-04	6.2777E-32
61.	2.9075E-07	2.9990E-07	2.9990E-07	3.3078E-02	0.00000	1.3078E-04	3.3078E-32
62.	2.8032E-07	2.8032E-07	2.8044E-07	7.2001E-02	0.00000	1.8044E-04	7.2001E-32
63.	2.7032E-07	2.6044E-07	2.6044E-07	7.4771E-02	0.00000	1.4144E-04	7.4771E-32
64.	2.5104E-07	2.5044E-07	2.5044E-07	9.7803E-02	0.00000	1.4004E-04	1.8783E-32
65.	2.2770E-07	2.0373E-07	2.0334E-07	2.1079E-01	0.00000	1.6042E-04	5.8778E-32
66.	1.6044E-07	1.6334E-07	1.6394E-07	2.5957E-01	0.00000	1.7011E-04	9.5043E-32
67.	1.4073E-07	1.2767E-07	1.2709E-07	2.8710E-01	0.00000	2.0397E-04	1.3071E-31
68.	1.1119E-07	9.6072E-08	9.5698E-08	3.0227E-01	0.00000	2.3197E-04	1.6810E-31
69.	9.1072E-08	6.9422E-08	6.8785E-08	3.4444E-01	0.00000	2.7608E-04	1.7267E-31
70.	5.6825E-08	4.9043E-08	4.9073E-08	2.6640E-01	0.00000	3.2470E-04	1.0389E-31
71.	4.2737E-08	3.6775E-08	3.6408E-08	3.3611E-01	0.00000	3.7039E-04	8.5164E-32
72.	3.0612E-08	2.5710E-08	2.5512E-08	4.0134E-01	0.00000	4.3316E-04	6.1790E-32
73.	2.0443E-08	1.6670E-08	1.6504E-08	5.0203E-01	0.00000	5.6628E-04	3.8116E-32
74.	1.2397E-08	9.6307E-09	9.6479E-09	6.7294E-01	0.00000	7.4663E-04	1.8742E-32
75.	6.3290E-09	4.9301E-09	4.9398E-09	1.0217E 00	0.00000	1.0993E-03	4.3813E-33
76.	2.2770E-09	1.5164E-09	1.5224E-09	3.1294E 00	0.00000	2.0114E-03	1.0640E-33
	1.0000E-10						

## APPENDIX II

### CARD IMAGE VERSION OF THE SIGMA MASTER TAPE AND THE PROGRAM MTBIN FOR GENERATION OF THE BINARY TAPE

The SIGMA MASTER TAPE normally used is a binary tape for the **Borroughs B6700** computer at **Riss**. Unfortunately a tape may now and then be spoiled by, for instance, a parity error, and it is therefore important to be able to regenerate it if necessary. The binary SIGMA MASTER TAPE is backed up by a card image version of the information which may also be used in transferring the library to another computer.

The card image version is filed on 3 magnetic tapes labelled **AEK133**, **AEK108**, and **AEK110** and containing a total of 78,806 cards. The format of the card image version is the same as for the binary tape described in section 9.1, except that a "record" now means the number of cards necessary to hold the information from a binary record. On each card the information is printed in the first 72 columns, and the remaining 8 are used for numbering of the cards.

All cards are printed in the format **6E12.5** except for the card containing the first record of the tape which has the format **4F12.0**, **X24**, and the first card for each new material which contains an alphanumeric variable and has therefore been given the format **3E12.5**, **X3**, **A6**, **X3**, **2E12.5**. Where a card is not fully utilized, the remaining places are filled up by noughts. In front of the tapes one card containing a heading is placed, and its text is

on **AEK133**: SIGMA MASTER TAPE PART 1

on **AEK108**: SIGMA MASTER TAPE PART 2

on **AEK110**: SIGMA MASTER TAPE PART 3

The card image tapes must be read with the file attributes

**MAXRECSIZE** = 14

**BLOCKSIZE** = 280

which means that the tapes are blocked with 20 cards in each block. The tapes are 9 track tapes in **EBCDIC**, written with the density 800BPI.

To generate the binary tape from the three **EBCDIC** tapes a small **ALGOL**-program, **MTBIN**, was written. The program has no card input,

so the only thing necessary to do before a run is that the binary output tape which is called FILMT internally in the program must be connected with the physical output tape. This is most easily done by inserting one card after the first BEGIN in the program with the text:

```
DEFINE FILMT = TAPENO # ;
```

The name TAPENO must be declared as follows:

```
FILE TAPENO (KIND = 14, MAXRECSIZE = 126, SAVEFACTOR = 999);
```

TAPENO will then be the label of the binary tape produced.



### APPENDIX III

#### MATERIALS AND PROCESSES IN THE UKNDL, VERSION 1968

In the following the contents of the UKNDL, version 1968, are listed. For each of the four files, files 1, 2, 3, and 5, the materials and processes are printed. A material is identified by its data file number, DFN, and described by the name following immediately after the DFN. The reactions given for each material are identified by the reaction type number of which the first digit is the general classification number, GCN, and the last three form the particular classification number, PCN, as explained in section 2.2.

For each reaction as well as for each material the number of records or cards is given.

CONTENTS OF GALAXY LIBRARY TAPE FILE NO 1

TOTAL 19933 RECORDS

OF MATERIAL RECORDS REACTION RECORDS

67	H	292	1001 1002 1003 1004 1005 1006 1007 1008 1009 1010 1011 1012 1013 1014 1015 1016 1017 1018 1019 1020 1021 1022 1023 1024 1025 1026 1027 1028 1029 1030 1031 1032 1033 1034 1035 1036 1037 1038 1039 1040 1041 1042 1043 1044 1045 1046 1047 1048 1049 1050 1051 1052 1053 1054 1055 1056 1057 1058 1059 1060 1061 1062 1063 1064 1065 1066 1067 1068 1069 1070 1071 1072 1073 1074 1075 1076 1077 1078 1079 1080 1081 1082 1083 1084 1085 1086 1087 1088 1089 1090 1091 1092 1093 1094 1095 1096 1097 1098 1099 1100 1101 1102 1103 1104 1105 1106 1107 1108 1109 1110 1111 1112 1113 1114 1115 1116 1117 1118 1119 1120 1121 1122 1123 1124 1125 1126 1127 1128 1129 1130 1131 1132 1133 1134 1135 1136 1137 1138 1139 1140 1141 1142 1143 1144 1145 1146 1147 1148 1149 1150 1151 1152 1153 1154 1155 1156 1157 1158 1159 1160 1161 1162 1163 1164 1165 1166 1167 1168 1169 1170 1171 1172 1173 1174 1175 1176 1177 1178 1179 1180 1181 1182 1183 1184 1185 1186 1187 1188 1189 1190 1191 1192 1193 1194 1195 1196 1197 1198 1199 1200 1201 1202 1203 1204 1205 1206 1207 1208 1209 1210 1211 1212 1213 1214 1215 1216 1217 1218 1219 1220 1221 1222 1223 1224 1225 1226 1227 1228 1229 1230 1231 1232 1233 1234 1235 1236 1237 1238 1239 1240 1241 1242 1243 1244 1245 1246 1247 1248 1249 1250 1251 1252 1253 1254 1255 1256 1257 1258 1259 1260 1261 1262 1263 1264 1265 1266 1267 1268 1269 1270 1271 1272 1273 1274 1275 1276 1277 1278 1279 1280 1281 1282 1283 1284 1285 1286 1287 1288 1289 1290 1291 1292 1293 1294 1295 1296 1297 1298 1299 1300 1301 1302 1303 1304 1305 1306 1307 1308 1309 1310 1311 1312 1313 1314 1315 1316 1317 1318 1319 1320 1321 1322 1323 1324 1325 1326 1327 1328 1329 1330 1331 1332 1333 1334 1335 1336 1337 1338 1339 1340 1341 1342 1343 1344 1345 1346 1347 1348 1349 1350 1351 1352 1353 1354 1355 1356 1357 1358 1359 1360 1361 1362 1363 1364 1365 1366 1367 1368 1369 1370 1371 1372 1373 1374 1375 1376 1377 1378 1379 1380 1381 1382 1383 1384 1385 1386 1387 1388 1389 1390 1391 1392 1393 1394 1395 1396 1397 1398 1399 1400 1401 1402 1403 1404 1405 1406 1407 1408 1409 1410 1411 1412 1413 1414 1415 1416 1417 1418 1419 1420 1421 1422 1423 1424 1425 1426 1427 1428 1429 1430 1431 1432 1433 1434 1435 1436 1437 1438 1439 1440 1441 1442 1443 1444 1445 1446 1447 1448 1449 1450 1451 1452 1453 1454 1455 1456 1457 1458 1459 1460 1461 1462 1463 1464 1465 1466 1467 1468 1469 1470 1471 1472 1473 1474 1475 1476 1477 1478 1479 1480 1481 1482 1483 1484 1485 1486 1487 1488 1489 1490 1491 1492 1493 1494 1495 1496 1497 1498 1499 1500 1501 1502 1503 1504 1505 1506 1507 1508 1509 1510 1511 1512 1513 1514 1515 1516 1517 1518 1519 1520 1521 1522 1523 1524 1525 1526 1527 1528 1529 1530 1531 1532 1533 1534 1535 1536 1537 1538 1539 1540 1541 1542 1543 1544 1545 1546 1547 1548 1549 1550 1551 1552 1553 1554 1555 1556 1557 1558 1559 1560 1561 1562 1563 1564 1565 1566 1567 1568 1569 1570 1571 1572 1573 1574 1575 1576 1577 1578 1579 1580 1581 1582 1583 1584 1585 1586 1587 1588 1589 1590 1591 1592 1593 1594 1595 1596 1597 1598 1599 1600 1601 1602 1603 1604 1605 1606 1607 1608 1609 1610 1611 1612 1613 1614 1615 1616 1617 1618 1619 1620 1621 1622 1623 1624 1625 1626 1627 1628 1629 1630 1631 1632 1633 1634 1635 1636 1637 1638 1639 1640 1641 1642 1643 1644 1645 1646 1647 1648 1649 1650 1651 1652 1653 1654 1655 1656 1657 1658 1659 1660 1661 1662 1663 1664 1665 1666 1667 1668 1669 1670 1671 1672 1673 1674 1675 1676 1677 1678 1679 1680 1681 1682 1683 1684 1685 1686 1687 1688 1689 1690 1691 1692 1693 1694 1695 1696 1697 1698 1699 1700 1701 1702 1703 1704 1705 1706 1707 1708 1709 1710 1711 1712 1713 1714 1715 1716 1717 1718 1719 1720 1721 1722 1723 1724 1725 1726 1727 1728 1729 1730 1731 1732 1733 1734 1735 1736 1737 1738 1739 1740 1741 1742 1743 1744 1745 1746 1747 1748 1749 1750 1751 1752 1753 1754 1755 1756 1757 1758 1759 1760 1761 1762 1763 1764 1765 1766 1767 1768 1769 1770 1771 1772 1773 1774 1775 1776 1777 1778 1779 1780 1781 1782 1783 1784 1785 1786 1787 1788 1789 1790 1791 1792 1793 1794 1795 1796 1797 1798 1799 1800 1801 1802 1803 1804 1805 1806 1807 1808 1809 1810 1811 1812 1813 1814 1815 1816 1817 1818 1819 1820 1821 1822 1823 1824 1825 1826 1827 1828 1829 1830 1831 1832 1833 1834 1835 1836 1837 1838 1839 1840 1841 1842 1843 1844 1845 1846 1847 1848 1849 1850 1851 1852 1853 1854 1855 1856 1857 1858 1859 1860 1861 1862 1863 1864 1865 1866 1867 1868 1869 1870 1871 1872 1873 1874 1875 1876 1877 1878 1879 1880 1881 1882 1883 1884 1885 1886 1887 1888 1889 1890 1891 1892 1893 1894 1895 1896 1897 1898 1899 1900 1901 1902 1903 1904 1905 1906 1907 1908 1909 1910 1911 1912 1913 1914 1915 1916 1917 1918 1919 1920 1921 1922 1923 1924 1925 1926 1927 1928 1929 1930 1931 1932 1933 1934 1935 1936 1937 1938 1939 1940 1941 1942 1943 1944 1945 1946 1947 1948 1949 1950 1951 1952 1953 1954 1955 1956 1957 1958 1959 1960 1961 1962 1963 1964 1965 1966 1967 1968 1969 1970 1971 1972 1973 1974 1975 1976 1977 1978 1979 1980 1981 1982 1983 1984 1985 1986 1987 1988 1989 1990 1991 1992 1993 1994 1995 1996 1997 1998 1999 2000 2001 2002 2003 2004 2005 2006 2007 2008 2009 2010 2011 2012 2013 2014 2015 2016 2017 2018 2019 2020 2021 2022 2023 2024 2025 2026 2027 2028 2029 2030 2031 2032 2033 2034 2035 2036 2037 2038 2039 2040 2041 2042 2043 2044 2045 2046 2047 2048 2049 2050 2051 2052 2053 2054 2055 2056 2057 2058 2059 2060 2061 2062 2063 2064 2065 2066 2067 2068 2069 2070 2071 2072 2073 2074 2075 2076 2077 2078 2079 2080 2081 2082 2083 2084 2085 2086 2087 2088 2089 2090 2091 2092 2093 2094 2095 2096 2097 2098 2099 2100 2101 2102 2103 2104 2105 2106 2107 2108 2109 2110 2111 2112 2113 2114 2115 2116 2117 2118 2119 2120 2121 2122 2123 2124 2125 2126 2127 2128 2129 2130 2131 2132 2133 2134 2135 2136 2137 2138 2139 2140 2141 2142 2143 2144 2145 2146 2147 2148 2149 2150 2151 2152 2153 2154 2155 2156 2157 2158 2159 2160 2161 2162 2163 2164 2165 2166 2167 2168 2169 2170 2171 2172 2173 2174 2175 2176 2177 2178 2179 2180 2181 2182 2183 2184 2185 2186 2187 2188 2189 2190 2191 2192 2193 2194 2195 2196 2197 2198 2199 2200 2201 2202 2203 2204 2205 2206 2207 2208 2209 2210 2211 2212 2213 2214 2215 2216 2217 2218 2219 2220 2221 2222 2223 2224 2225 2226 2227 2228 2229 2230 2231 2232 2233 2234 2235 2236 2237 2238 2239 2240 2241 2242 2243 2244 2245 2246 2247 2248 2249 2250 2251 2252 2253 2254 2255 2256 2257 2258 2259 2260 2261 2262 2263 2264 2265 2266 2267 2268 2269 2270 2271 2272 2273 2274 2275 2276 2277 2278 2279 2280 2281 2282 2283 2284 2285 2286 2287 2288 2289 2290 2291 2292 2293 2294 2295 2296 2297 2298 2299 2300 2301 2302 2303 2304 2305 2306 2307 2308 2309 2310 2311 2312 2313 2314 2315 2316 2317 2318 2319 2320 2321 2322 2323 2324 2325 2326 2327 2328 2329 2330 2331 2332 2333 2334 2335 2336 2337 2338 2339 2340 2341 2342 2343 2344 2345 2346 2347 2348 2349 2350 2351 2352 2353 2354 2355 2356 2357 2358 2359 2360 2361 2362 2363 2364 2365 2366 2367 2368 2369 2370 2371 2372 2373 2374 2375 2376 2377 2378 2379 2380 2381 2382 2383 2384 2385 2386 2387 2388 2389 2390 2391 2392 2393 2394 2395 2396 2397 2398 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			2248	1228	1239	3
			2249	1229	1240	3
			2250	1230	1241	3
			2251	1231	1242	3
			2252	1232	1243	3
			2253	1233	1244	3
			2254			



CONTENTS OF GALAXY LIBRARY TAPE FILE NO 3

1974 12003 RECORDS

OF MATERIAL RECORDS REACTION RECORDS

220	475	195	1001	20	1016
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			1021	20	1036
			1022	20	1037
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			1037	20	1052
			1038	20	1053
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			1107	20	1122
			1108	20	1123
			1109	20	1124
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225	0059	71	1103	30
226	0150	20	1109	69
			1014	10
			1109	27
227	0063	71	1014	10
			1109	30
208	700	7	1014	5
234	2690	12	1016	10
204	00103	12	1014	10
230	10115	27	1009	25
200	1127	13	1014	11
209	70160	4	1014	6
210	60175	9	1014	6
172	001	12	1001	3
			1009	3
			2009	5
55	1/4	15	1001	3
			1009	3
			2009	5
56	5641	12	1001	3
			1009	3
			2009	5
151	600	15	1001	3
			1009	3
			2009	5

CONTENTS OF GALAXY LIBRARY TAPE FILE NO. 5

TOTAL		6537 RECORDS		OPM MATERIAL RECORDS REACTION RECORDS	
701	8041	88	1109	86	
702	8042	88	1109	86	
703	8051	80	1109	78	
704	8044	86	1109	78	
705	8055	80	1109	78	
706	8045	80	1109	78	
707	8046	85	1109	78	
708	8047	83	1109	81	
709	8088	88	1109	86	
710	8409	88	1109	86	
711	709	83	1109	81	
712	3496	83	1109	81	
713	740	88	1109	81	
714	701	88	1109	86	
715	2491	83	1109	81	
716	2492	83	1109	81	
717	2493	88	1109	86	
718	2494	82	1109	80	
719	4095	80	1109	78	
720	4096	82	1109	80	
721	4097	80	1109	78	
722	4098	80	1109	78	
723	4099	83	1109	81	
724	80100	80	1109	78	
725	80101	80	1109	78	
726	80102	80	1109	78	
727	80103	80	1109	78	
728	80104	80	1109	78	
729	80105	88	1109	78	

730	PM105	80	1109	86	
731	PM106	80	1109	78	
732	PM107	80	1109	78	
733	PM108	80	1109	78	
734	46109	80	1109	78	
735	CM111	80	1109	78	
736	46115	80	1109	78	
737	58125	80	1109	78	
738	1127	80	1109	78	
739	7E128	43	1109	41	
740	1129	80	1109	78	
741	7E130	43	1109	81	
742	1131	80	1109	86	
743	4E131	80	1109	78	
744	4E132	82	1109	80	
745	4E133	80	1109	86	
746	CS133	80	1109	78	
747	4E134	82	1109	80	
748	CS134	88	1109	86	
749	1135	88	1109	86	
750	4E135	88	1109	86	
751	CS135	80	1109	78	
752	4E136	83	1109	81	
753	CS137	88	1109	86	
754	4E136	85	1109	81	
755	4A139	87	1109	80	
756	CL140	80	1109	78	
757	4C141	80	1109	78	
758	CL142	82	1109	80	
759	80143	48	1109	86	
760	80144	83	1109	81	
761	80145	85	1109	78	
762	80146	83	1109	81	
763	PM147	85	1109	81	

764	003140	00	1109	70
765	04140	00	1109	70
766	04140	00	1109	06
767	04140	00	1109	06
768	003140	00	1109	70
769	04150	00	1109	01
770	04151	00	1109	06
771	04152	00	1109	70
772	04153	00	1109	70
773	04154	00	1109	70
774	04154	00	1109	06
775	04155	00	1109	70
776	00155	00	1109	06
777	00156	00	1109	70
778	00157	00	1109	70